A Simple Variational Principle for Synchrotron Radiation

With Applications to Small-Bunch Undulator Radiation

A.E. Charman*

with G. Penn◇ and J.S. Wurtele*

*U.C. Berkeley Department of Physics

◇Center for Beam Physics, Lawrence Berkeley National Laboratory

IOTA Collaboration Meeting

06/17/2020

In memory of our friend and colleague Max S. Zolotorev (1941–2020)

- Max taught us many interesting ideas, including some directly and indirectly relevant to the variational principle discussed in this talk

- consider "Max-wellian" perspectives on particle acceleration
  - relate the energy exchange with the interference between drive fields and radiation fields
  - exploit connections between far-field behavior and near-field physics
- *formation length* and *formation time* are fundamental scales
  - Wiezsacker-Williams approximation can be applied to classical radiation processes
  - think carefully about what is happening as charges "shake loose" clouds of virtual photons
- sometimes the noise in radiation is the signal
  - e.g., fluctuational tomography
  - even classical electromagnetism reveals veins which are rich, deep, and far from tapped
- and many more lessons both clever and profound
  - optical stochastic cooling
  - slicing
  - etc….

Variational Principles are Perhaps Better Known in Classical and Quantum Mechanics But Are Ubiquitous in Electromagnetism

- *Thomson's*, *Dirichlet's*, and *Hadamard's* Principles in electrostatics
- *Reciprocity* relations and *reaction* principles in waveguide, cavity, aperture, and antenna problems
- Raleigh, Ritz, Galerkin, finite element, minimum residual, etc. and related *numerical methods*
- *Fermat's Principle* and *Hamilton's* formalism in ray optics
- *Maximum entropy* and *minimum free energy* principles in radiation thermodynamics
- *Action* principles in Lagrangian/Hamiltonian formulations of electrodynamics
- *Schwinger* variational principles for transmission lines, waveguides, scattering
- specialized variational principles for lasers and undulators (e.g. Xie)

Advantages of Variational Principles are Well Known

- unified theoretical treatments
- compact mathematical descriptions
- coordinate changes are simplified, constraints easily imposed, conservation laws incorporated
- appealing physical interpretations often suggested
- classical/quantum connections are more readily apparent
- starting points for efficient approximation or numerical computation:

  systems of complicated PDEs or integro-differential equations may be replaced with more tractable quadratures, ODEs, algebraic or perhaps even linear equations, and/or ordinary function minimization....

Motivation for the Maximum "Power" Variational Principle (MPVP)

- results were derived in the context of synchrotron radiation from relativistic electron beams in undulators
  - but directly applicable to general "magnetic Bremsstrahlung" situations –bending magnets, wigglers, undulators, etc.…
  - after suitable generalization, *should* also be relevant to cases of Cerenkov, transition, waveguide, Smith-Purcell, CSR, or other types of radiation…
- practical approximation technique—at least in important special case of paraxial radiation fields
  - has been successfully applied to an analysis of x-ray generation via harmonic cascade in sequenced modulating/radiating undulators
- variational approximation principle provides estimate for spatial and polarization profile and lower bound on radiated spectrum
  - given the sources, provides alternative to solving for fields via Lienard-Wiechert potentials, Heaviside-Feynman, Jeffimenko, Panofsky, or related expressions, or to making Wilcox-type series expansions, or using Fresnel diffraction integrals

Assumptions/Applicability

- classical radiation arising from charges following *prescribed* classical spatiotemporal trajectories
  - radiation reaction/recoil, multiple scattering, gain, absorption. or other feedback of the radiation on the charges is negligible—often reasonable for relativistic beams....
  - stimulated-emission component of radiation must remains small compared to spontaneous emission component
  - radiation fields are classical according to Glauber-Sudarshan criterion
- trajectories are uniquely determined by initial conditions, external EM fields (wigglers, bending magnets, quadrupoles, cavities, etc.) and possibly space-charge self-fields (either exact Coulomb fields or a mean-field/Vlasov treatment)
  - no gain or self-consistent recoil/bunching
  - but arbitrary pre-bunching would be allowed
- sources are localized in space (so far-field is defined)
- sources are at least weakly localized in time (so Fourier transforms exist)
- after emission, radiation otherwise propagates in free space
  - but could be subsequently transported through passive optical devices (lenses, mirrors)

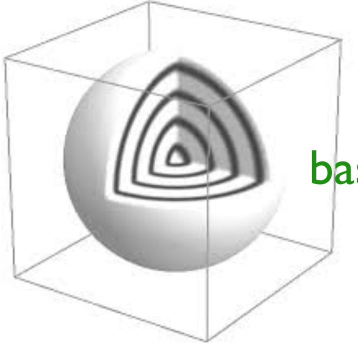
Maximum Power Variational Principle for Spontaneous Wiggler Radiation

Summary and Strategy:

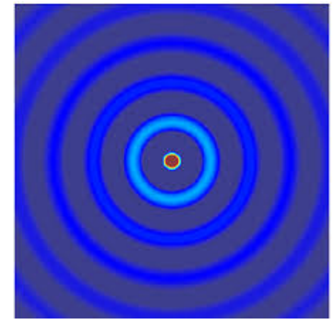
- radiative EM fields are analyzed in a Hilbert-space settings
  - paraxial case is well known given formal equivalence between paraxial optics and non-relativistic, single-particle quantum mechanics
  - but can be generalized to non-paraxial fields in full 3D geometry...
  - to ensure normalizability, inner products are related to Poynting fluxes rather than field energies, since the latter can diverge badly for monochromatic harmonic sources
- fields emitted from prescribed sources, satisfying an inhomogeneous wave equation with outgoing Sommerfeld boundary conditions, are uniquely decomposed into irrotational, reactive, and radiation components
- field propagation described formally by Green function techniques
- using Poynting's theorem/energy-conservation, various reciprocity, hermiticity, and surjectivity properties of these Green functions, and positive-definiteness of the relevant Hilbert-space inner products, a variational principle is derived, saying, in effect, that

> classical charges radiate spontaneously "as much as possible," consistent with energy conservation

7



Basic Formalism



based on decomposing into irrotational, reactive and radiative fields

start in frequency domain and Coulomb gauge

$$\left(\nabla^2 + k^2\right) \boldsymbol{A}_\perp(\boldsymbol{x};\omega) = -\mu_0\, \boldsymbol{J}_\perp(\boldsymbol{x};\omega) \qquad \boldsymbol{\nabla}\cdot\boldsymbol{A}_\perp(\boldsymbol{x};\omega) = 0$$

relevant source is solenoidal part of current

$$\boldsymbol{J}(\boldsymbol{x};\omega) = \boldsymbol{J}_\perp(\boldsymbol{x};\omega) + \boldsymbol{J}_\parallel(\boldsymbol{x};\omega) \qquad \boldsymbol{\nabla}\cdot\boldsymbol{J}_\perp(\boldsymbol{x};\omega) = 0 \qquad \boldsymbol{\nabla}\times\boldsymbol{J}_\parallel(\boldsymbol{x};\omega) = \boldsymbol{0}$$

formal solution is expressible in terms of Green functions

$$\boldsymbol{A}_\perp(\boldsymbol{x};\omega) = \boldsymbol{A}_{\rm in}(\boldsymbol{x};\omega) + \boldsymbol{A}_{\rm ret}(\boldsymbol{x};\omega) = \boldsymbol{A}_{\rm in}(\boldsymbol{x};\omega) + \mu_0 \int d^3\boldsymbol{x}'\, G_{\rm ret}(\boldsymbol{x};\boldsymbol{x}';\omega)\, \boldsymbol{J}_\perp(\boldsymbol{x}';\omega)$$

$$\boldsymbol{A}_\perp(\boldsymbol{x};\omega) = \boldsymbol{A}_{\rm out}(\boldsymbol{x};\omega) + \boldsymbol{A}_{\rm adv}(\boldsymbol{x};\omega) = \boldsymbol{A}_{\rm out}(\boldsymbol{x};\omega) + \mu_0 \int d^3\boldsymbol{x}'\, G_{\rm adv}(\boldsymbol{x};\boldsymbol{x}';\omega)\, \boldsymbol{J}_\perp(\boldsymbol{x}';\omega)$$

$$\boldsymbol{A}_{\rm rad}(\boldsymbol{x};\omega) = \boldsymbol{A}_{\rm out}(\boldsymbol{x};\omega) - \boldsymbol{A}_{\rm in}(\boldsymbol{x};\omega) = \boldsymbol{A}_{\rm ret}(\boldsymbol{x};\omega) - \boldsymbol{A}_{\rm adv}(\boldsymbol{x};\omega) = 2\mu_0 \int d^3\boldsymbol{x}'\, D(\boldsymbol{x};\boldsymbol{x}';\omega)\, \boldsymbol{J}_\perp(\boldsymbol{x}';\omega)$$

$$G_{\rm ret}(\boldsymbol{x},\boldsymbol{x}';\omega) = \frac{e^{+ik|\boldsymbol{x}-\boldsymbol{x}'|}}{4\pi\,|\boldsymbol{x}-\boldsymbol{x}'|}$$

casual/retarded/outgoing
Green function

both satisfy

$$\left(\nabla^2 + k^2\right) G(\boldsymbol{x},\boldsymbol{x}';\omega) = -\delta(\boldsymbol{x}-\boldsymbol{x}')$$

$$G_{\rm adv}(\boldsymbol{x},\boldsymbol{x}';\omega) = \frac{e^{-ik|\boldsymbol{x}-\boldsymbol{x}'|}}{4\pi\,|\boldsymbol{x}-\boldsymbol{x}'|}$$

acausal/advanced/ingoing/time-reversed
Green function

$$D(\boldsymbol{x},\boldsymbol{x}';\omega) = \tfrac{1}{2}\left[\, G_{\rm ret}(\boldsymbol{x},\boldsymbol{x}';\omega) - G_{\rm adv}(\boldsymbol{x},\boldsymbol{x}';\omega)\,\right] = \frac{i\,\sin k\,|\boldsymbol{x}-\boldsymbol{x}'|}{4\pi\,|\boldsymbol{x}-\boldsymbol{x}'|}$$

radiation kernel satisfies the source-free Helmholtz equation $\left(\nabla^2 + k^2\right) D(\boldsymbol{x},\boldsymbol{x}';\omega) = 0$

Solenoidal Radiative and Reactive Fields

can decompose solenoidal causal/retarded EM fields into "reactive" near fields plus radiation fields

$$\boldsymbol{A}_{\text{ret}}(\boldsymbol{x};\omega) = \bar{\boldsymbol{A}}(\boldsymbol{x};\omega) + \tfrac{1}{2}\boldsymbol{A}_{\text{rad}}(\boldsymbol{x};\omega)$$

using corresponding decomposition of Green function: $G_{\text{ret}}(\boldsymbol{x},\boldsymbol{x}';\omega) = \bar{G}(\boldsymbol{x},\boldsymbol{x}';\omega) + D(\boldsymbol{x},\boldsymbol{x}';\omega)$

where

$$\bar{\boldsymbol{A}}(\boldsymbol{x};\omega) = \mu_0 \int d^3\boldsymbol{x}'\, \bar{G}(\boldsymbol{x};\boldsymbol{x}';\omega)\, \boldsymbol{J}_\perp(\boldsymbol{x}';\omega)$$

solenoidal "reactive" near fields

$$\boldsymbol{A}_{\text{rad}}(\boldsymbol{x};\omega) = 2\mu_0 \int d^3\boldsymbol{x}'\, D(\boldsymbol{x};\boldsymbol{x}';\omega)\, \boldsymbol{J}_\perp(\boldsymbol{x}';\omega)$$

"Dirac" radiation fields

$$\bar{G}(\boldsymbol{x},\boldsymbol{x}';\omega) = \tfrac{1}{2}\left[\, G_{\text{ret}}(\boldsymbol{x},\boldsymbol{x}';\omega) + G_{\text{adv}}(\boldsymbol{x},\boldsymbol{x}';\omega)\,\right] = \frac{\cos k\,|\boldsymbol{x}-\boldsymbol{x}'|}{4\pi\,|\boldsymbol{x}-\boldsymbol{x}'|}$$

half-advanced/half-retarded, or "principal value" Green function

$$D(\boldsymbol{x},\boldsymbol{x}';\omega) = \tfrac{1}{2}\left[\, G_{\text{ret}}(\boldsymbol{x},\boldsymbol{x}';\omega) - G_{\text{adv}}(\boldsymbol{x},\boldsymbol{x}';\omega)\,\right] = \frac{i\,\sin k\,|\boldsymbol{x}-\boldsymbol{x}'|}{4\pi\,|\boldsymbol{x}-\boldsymbol{x}'|}$$

radiation kernel

all source-free radiative solutions to the microscopic, free-space Maxwell's equations can be written (non-niquely) in terms of a convolution of the radiation kernel with *some* effective source

or (uniquely) in terms of a Kirchhoff diffraction integral over the outgoing far-fields ("radiation pattern")

Radiation and Radiation Fields

What do we mean? What should we mean?

- fields that have been "*shaken loose*" from the emitting charges and take on an independent existence
  - should solve the *source-free* Maxwell equations everywhere, including on the actual worldlines of sources
- can (*irreversibly*) *transport* energy, linear and angular momentum, and information "to infinity"
- depend on *acceleration* of source charges, not just velocities and positions
- can be expressed as superpositions of *null fields* (with vanishing invariants)
- in the *asymptotic far field, radiative* emission from one source charge:
  - exhibits $O(1/r)$ fall-off in distance between observation and emission points
  - electric and magnetic fields will be perpendicular to each other and to line of sight between point of emission and observation
  - satisfies outgoing Sommerfeld or Silver-Muller radiation conditions ???
- we adopt Dirac's definition of radiation fields associated with sources
  - difference between retarded and advanced fields in 3D geometry
  - difference between downstream and upstream fields in paraxial approximation
  - accounts for *finite* radiation reaction forces, in contrast to longitudinal and reactive fields, which lead to an infinite mass renormalization
  - accounts for actual *radiated* power as calculated by Larmor-Lienard formula
  - satisfies all of the above properties, except includes ingoing *and* outgoing (or upstream and downstream) components to cancel singularity at location of sources

Inner Products (Non-Paraxial Case)

volumetric, or "Joule" functional inner product:

$$\big\langle \boldsymbol{E}_\perp \big| \boldsymbol{J}'_\perp \big\rangle = \big\langle \boldsymbol{E}_\perp \big| \boldsymbol{J}' \big\rangle = \int_{\mathbb{R}^3} d^3\boldsymbol{x}\, \boldsymbol{E}_\perp(\boldsymbol{x};\omega)^* \cdot \boldsymbol{J}(\boldsymbol{x};\omega')$$

far-field surface, or "Poynting" product:

$$\big(\boldsymbol{E}, \boldsymbol{B}'\big) = \lim_{R\to\infty} R^2 \int_{r=R} d^2\Omega(\hat{\boldsymbol{r}})\ \hat{\boldsymbol{r}} \cdot \big[\, \boldsymbol{E}(r\hat{\boldsymbol{r}};\omega)^* \times \boldsymbol{B}'(r\hat{\boldsymbol{r}};\omega')\, \big]$$

various manipulations lead to the important Poynting relations

$$-\operatorname{Re}\big\langle \boldsymbol{E}_{\mathrm{ret}} \big| \boldsymbol{J} \big\rangle = \tfrac{1}{\mu_0} \operatorname{Re}\big(\boldsymbol{E}_{\mathrm{ret}}, \boldsymbol{B}_{\mathrm{ret}}\big) = \tfrac{1}{\mu_0}\big(\boldsymbol{E}_{\mathrm{ret}}, \boldsymbol{B}_{\mathrm{ret}}\big) \geq 0$$

$$-\operatorname{Re}\big\langle \boldsymbol{E}_{\mathrm{adv}} \big| \boldsymbol{J} \big\rangle = \tfrac{1}{\mu_0} \operatorname{Re}\big(\boldsymbol{E}_{\mathrm{adv}}, \boldsymbol{B}_{\mathrm{adv}}\big) = \tfrac{1}{\mu_0}\big(\boldsymbol{E}_{\mathrm{adv}}, \boldsymbol{B}_{\mathrm{adv}}\big) = -\tfrac{1}{\mu_0}\big(\boldsymbol{E}_{\mathrm{ret}}, \boldsymbol{B}_{\mathrm{ret}}\big) \leq 0$$

and conjugate-reciprocity relations

$$\big\langle \boldsymbol{E}_{\mathrm{rad}} \,\big|\, \boldsymbol{J}'_\perp \big\rangle = \big\langle \boldsymbol{J}_\perp \,\big|\, \boldsymbol{E}'_{\mathrm{rad}} \big\rangle = \big\langle \boldsymbol{E}'_{\mathrm{rad}} \,\big|\, \boldsymbol{J}_\perp \big\rangle^*$$

Explicit Representation of 3D Hilbert Space

Hilbert spaces for outgoing, ingoing, and radiation solenoidal vector fields may be explicitly defined via expansions in spherical waves (multipoles):

$$\boldsymbol{A}_\perp(\boldsymbol{x};\omega) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\left\{a^E_{\ell m}(\omega)\,\tfrac{1}{ik}\boldsymbol{\nabla}\times[f_\ell(kr)\,\boldsymbol{X}_{\ell m}(\hat{\boldsymbol{r}})] + a^M_{\ell m}(\omega)\,f_\ell(kr)\,\boldsymbol{X}_{\ell m}(\hat{\boldsymbol{r}})\right\}$$

$$f_\ell(kr) = \begin{cases} h^{(1)}(kr) & \propto \frac{e^{+ikr}}{kr} \\ h^{(2)}(kr) & \propto \frac{e^{-ikr}}{kr} \\ 2i\,j_\ell(kr) & \propto \frac{\sin kr}{kr} \end{cases}$$

spherical Hankel function of 1st kind for **retarded** fields

spherical Hankel function of 2nd kind for **advanced** fields

spherical Bessel function for **radiation** fields

$$\frac{1}{i\sqrt{\ell(\ell+1)}}\,\boldsymbol{x}\times\boldsymbol{\nabla}Y_{\ell\,m}(\hat{\boldsymbol{r}})$$ = vector spherical harmonics (related to "Hansen multipoles")

$$G_{\rm ret}(\boldsymbol{x},\boldsymbol{x}';\omega) = \sum_{\ell=0}^{\infty} j_\ell(kr_<)\,h^-_\ell(kr_>)\sum_{m=-\ell}^{+\ell} Y_{\ell m}(\hat{\boldsymbol{r}}')^*\,Y_{\ell m}(\hat{\boldsymbol{r}})$$

retarded Green function

radiation Kernel

$$D(\boldsymbol{x},\boldsymbol{x}';\omega) = i\sum_{\ell=0}^{\infty} j_\ell(kr')\,j_\ell(kr)\sum_{m=-\ell}^{+\ell} Y_{\ell m}(\hat{\boldsymbol{r}}')^*\,Y_{\ell m}(\hat{\boldsymbol{r}})$$

$$\tfrac{1}{\mu_0}(\boldsymbol{E},\boldsymbol{B}') = \tfrac{c}{\mu_0}\sum_\ell\sum_m\left[a^E_{\ell m}(\omega)^*{a^E}'_{\ell m}(\omega) + a^M_{\ell m}(\omega)^*{a^M}'_{\ell m}(\omega)\right]$$

Poynting inner product (proportional to the spectral density of outgoing Poynting flux in the asymptotic far field) is expressible in terms of the ordinary l^2 inner product of the multipole expansion coefficients

Poynting Inequalities and Variational Principle

further algebraic manipulations reveal

$$-\tfrac{1}{2}\,\mathrm{Re}\big\langle \boldsymbol{E}_{\mathrm{rad}}\big|\boldsymbol{J}\big\rangle = \tfrac{1}{\mu_0}\big(\boldsymbol{E}_{\mathrm{ret}}, \boldsymbol{B}_{\mathrm{ret}}\big) \geq 0$$

$$\tfrac{1}{\mu_0}\big(\boldsymbol{E}_{\mathrm{ret}}, \boldsymbol{B}_{\mathrm{ret}}\big) \geq -\tfrac{1}{\mu_0}\big(\boldsymbol{e}_{\mathrm{ret}}, \boldsymbol{b}_{\mathrm{ret}}\big) - \mathrm{Re}\big\langle \boldsymbol{e}_{\mathrm{rad}}\big|\boldsymbol{J}\big\rangle$$

upper-case = “true” fields

lower-case = “trial” fields

which in turn implies a variational principle in the form

$$\tfrac{1}{\mu_0}\big(\boldsymbol{E}_{\mathrm{ret}}, \boldsymbol{B}_{\mathrm{ret}}\big) \geq \max_{\boldsymbol{\alpha}}\big[\tfrac{1}{\mu_0}\big(\boldsymbol{e}_{\mathrm{ret}}, \boldsymbol{b}_{\mathrm{ret}}\big)\big]$$

such that: $\tfrac{1}{\mu_0}\big(\boldsymbol{e}_{\mathrm{ret}}, \boldsymbol{b}_{\mathrm{ret}}\big) = -\tfrac{1}{2}\,\mathrm{Re}\big\langle \boldsymbol{e}_{\mathrm{rad}}\big|\boldsymbol{J}\big\rangle$

and: $\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\boldsymbol{e}_{\mathrm{rad}}(\boldsymbol{x};\omega;\boldsymbol{\alpha}) = k^2\,\boldsymbol{e}_{\mathrm{rad}}(\boldsymbol{x};\omega;\boldsymbol{\alpha})$

Maximum "Power" Variational Principle (MPVP)

- Given a parameterized family of trial radiation modes
  - must be solenoidal solutions to source-free wave-equation at all frequencies of interest
  - variational parameters should determine the overall amplitude, phase, shape, and polarization of the trial mode, separately at each frequency
- parameters are to be estimated formally by maximizing spectral density of outgoing energy flux in far field
- or equivalently, by maximizing spectral density of work that *would* be exchanged between sources and radiation fields
- subject to a constraint enforcing energy conservation, saying that those integrals are equal (apart from a factor of 2)
  - in practice, polarization and relative profile can be optimized first, then overall amplitude can be determined using the energy conservation constraint
  - factor of $1/2$ arises to avoid over-counting in the energetics;
  - radiative analog of the factor of $1/2$ which occurs in the expression for the potential energy of a given charge distribution in electrostatics
  - "virtual" energy exchange is calculated between sources and source-free trial fields, even though only outgoing fields and near fields are actually present.

$$\frac{1}{\mu_0}\big(\boldsymbol{E}_{\mathrm{ret}}, \boldsymbol{B}_{\mathrm{ret}}\big) \geq \max_{\boldsymbol{\alpha}}\Big[\frac{1}{\mu_0}\big(\boldsymbol{e}_{\mathrm{ret}}, \boldsymbol{b}_{\mathrm{ret}}\big)\Big]$$

such that:
$$\frac{1}{\mu_0}\big(\boldsymbol{e}_{\mathrm{ret}}, \boldsymbol{b}_{\mathrm{ret}}\big) = -\tfrac{1}{2}\,\mathrm{Re}\big\langle \boldsymbol{e}_{\mathrm{rad}} \big| \boldsymbol{J}\big\rangle$$

and:
$$\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\boldsymbol{e}_{\mathrm{rad}}(\boldsymbol{x};\omega;\boldsymbol{\alpha}) = k^2\,\boldsymbol{e}_{\mathrm{rad}}(\boldsymbol{x};\omega;\boldsymbol{\alpha})$$

Paraxial Regime

applies to most undulator radiation and many other relativistic sources

light propagation predominately along $+\hat{\boldsymbol{z}}$ axis,

with characteristic diffraction angle $\Theta \sim \frac{1}{k\sigma} \ll 1$

$\boldsymbol{A}_\perp(\boldsymbol{x};\omega) = \boldsymbol{\psi}(\boldsymbol{x}_\perp, z;\omega)\, e^{+ikz}$ *slowly-varying envelope modulating carrier*

$[2ik\frac{\partial}{\partial z} + \nabla_\perp^2]\boldsymbol{\psi}(\boldsymbol{x}_\perp, z;\omega) = (1 - \hat{\boldsymbol{z}}\hat{\boldsymbol{z}}^{\mathrm{T}})e^{-ikz}\boldsymbol{J}_\perp(\boldsymbol{x}_\perp, z;\omega)$ *paraxial propagation equation*

$$\hat{\boldsymbol{z}} \cdot \boldsymbol{\psi}(\boldsymbol{x}_\perp, z;\omega) = 0$$

lowest-order gauge condition

$$[ik\hat{\boldsymbol{z}} + \boldsymbol{\nabla}_\perp] \cdot \boldsymbol{\psi}(\boldsymbol{x}_\perp, z;\omega) = 0$$

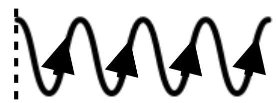
next-order gauge condition

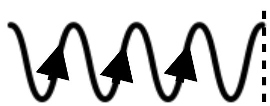
note that source-free fields are uniquely determined everywhere from transverse components in any one transverse plane

$[+i\frac{\partial}{\partial z} + \frac{1}{2k}\nabla_\perp^2]G(\boldsymbol{x}, \boldsymbol{x}';\omega) = i\,\delta(z - z')\,\delta(\boldsymbol{x}_\perp - \boldsymbol{x}'_\perp)$ **(using QM sign and phase conventions)**

$G_\pm(\boldsymbol{x}_\perp, z, \boldsymbol{x}'_\perp, z';\omega) = \pm\Theta(\pm[z - z'])\,\frac{k}{2\pi i[z-z']}\,e^{\frac{+ik\ |\boldsymbol{x}_\perp - \boldsymbol{x}'_\perp|^2}{2[z-z']}}$ *Green function/propagator/ Fresnel diffraction kernel*

downstream (+) Green function replaces retarded 3D Green function





upstream (–) Green function replaces retarded 3D Green function

rightward radiation fields are defined as differences between downstream and upstream fields, and are uniquely determined by the profile in any one transverse plane

$$\frac{1}{\mu_0}(\boldsymbol{E}, \boldsymbol{B})_\Theta = \frac{\omega^2}{c\mu_0} \lim_{Z\to\infty}\Big[+ \int\limits_{z=+Z} d^2\boldsymbol{x}_\perp\, |\boldsymbol{\psi}(\boldsymbol{x}_\perp, z;k)|^2 - \int\limits_{z=-Z} d^2\boldsymbol{x}_\perp\, |\boldsymbol{\psi}(\boldsymbol{x}_\perp, z;k)|^2 \Big]$$

analogous variational principles hold, at leading order and at next order in the paraxial expansion

15

Time Domain

- MPVP applies in the (positive) frequency domain
  - locally at each frequency of interest
  - or integrated over any frequency band
  - negative frequency components deducible from constraints arising from Cartesian components of physical fields being real-valued
- also applies globally (in an integrated sense) in the time domain
  - follows from the frequency-domain version, by unitary Fourier transformations and Parseval-Plancherel type identities
  - or can be derived directly, by arguments similar to those used in frequency domain
- time domain highlights different character of irrotational fields, reactive fields, and radiative fields
  - irrotational electric fields are just instantaneous Coulomb fields, strongly tied to source charges:

$$-\int dt \int d^3\boldsymbol{x}\, \boldsymbol{J}_{\parallel}(\boldsymbol{x},t)\cdot \boldsymbol{E}_{\parallel}(\boldsymbol{x},t) = \tfrac{1}{2}\int d^3\boldsymbol{x}\, \rho(\boldsymbol{x},t)\, \phi(\boldsymbol{x},t)^2 \,\Big|_{t=-\infty}^{t=+\infty}$$

  - reactive solenoidal fields represent near or intermediate-zone fields, which can temporarily exchange energy with sources or other fields, but not irreversibly transport energy to infinity:

$$\mathrm{P}\!\int dt \int d^3\boldsymbol{x}\; \boldsymbol{J}_{\perp}(\boldsymbol{x},t)\cdot \bar{\boldsymbol{E}}_{\perp}(\boldsymbol{x},t) = 0,$$

  - only radiation fields contribute to far-field Poynting flux:

$$-\tfrac{1}{2}\int dt \int d^3\boldsymbol{x}\, \boldsymbol{J}_{\perp}(\boldsymbol{x},t)\cdot \boldsymbol{E}_{\mathrm{rad}}(\boldsymbol{x},t) = \tfrac{1}{\mu_0}\lim_{R\to\infty}\int_{r=R} R^2\, d^2\Omega(\hat{\boldsymbol{r}})\; \hat{\boldsymbol{r}}\cdot\left[\,\boldsymbol{E}_{\mathrm{ret}}(r\hat{\boldsymbol{r}};t)\times \boldsymbol{B}_{\mathrm{ret}}(r\hat{\boldsymbol{r}};t)\,\right]$$

16

MPVP Optimization

- After optimization, the trial radiation fields are the best guess to the actual radiation fields within the parameterized family of source-free solutions considered
- outgoing far-field components approximate the outgoing fields radiated by the actual sources
- optimized power spectrum provides a variational lower bound for the actual power spectrum
  - at each frequency separately
  - or over any frequency band
- "power" is a bit of a misnomer
  - variational bound applies directly to spectral density of radiated energy
  - but variational functionals start with integrands related to work exchange and Poynting flux, not to electromagnetic energy density
- accuracy of approximated field profile and radiated power will (monotonically) improve as additional functionally-independent adjustable parameters are included
  - variational parameters may appear linearly (e.g., expansion coefficients in some fixed Gauss-Hermite or Gauss-Laguerre basis) and/or non-linearly (e.g., a spot size or waist location in a Gaussian mode)
  - but averaging over any statistical uncertainty in the particle trajectories constituting the source and performing the variational optimization do not in general commute

Some Interpretations of the MPVP

- maximizes the radiated power, consistent with this energy arising from work extractable from the actual sources
- minimizes a Hilbert-space "Poynting" distance between the actual radiation fields and the trial field within a parameterized family, of source-free solutions to Maxwell's equations
- in special cases, can be seen as an orthogonal projection of actual solution into manifold of trial solutions
- maximizes (for each harmonic component separately, or overall in time) spatial overlap/correlation, or physical resemblance, between the actual sources and radiation fields (as extrapolated back into the region of the sources via source-free propagation)
- reveals field shape which, if incident on sources, would maximally couple to them, and would experience maximum small-signal gain

18

Comparison to Madey's Theorem

In FEL amplifier or other stimulated emission problems, one naturally expects to observe, in the presence of gain, that mode which grows fastest

this idea is actually also applicable to the spontaneous emission regime...

arguments along lines of Einstein's derivation of *A* and *B* coefficients or its generalization to FEL physics in the form of Madey's theorem lead to definite connections between spontaneous emission, stimulated emission, and stimulated absorption, even when the radiation is entirely classical....

MPVP can be seen to be maximizing the mode shape for small-signal gain (without any saturation or back-action), with this "virtual" gain delivered proportional to the estimated power spontaneously radiated

really the only difference is: in the present case, by assuming prescribed sources we ignore radiation reaction, scattering, or any other feedback, so once emitted radiation cannot cause recoil or be subsequently scattered/absorbed by other parts of the source downstream...

hence under the assumptions of the MPVP it follows that:

$$\text{small-signal gain} \propto \text{``bare'' stimulated emission} \propto \text{ spontaneous emission}$$

while in the case of FELs, where feedback is essential, Madey's theorem says

$$\begin{gathered}\text{small-signal gain} \propto \text{``net'' stimulated emission} \\ \propto (\text{``bare'' stimulated emission} - \text{stimulated absorption}) \sim \tfrac{\partial}{\partial\omega}\, \text{spontaneous emission}\end{gathered}$$

Comparisons to Other Variational Principles

MPVP is reminiscent of, but distinct from, other well known variational principles used in electrostatics and circuit theory (Thomson and Dirchlet's principle); optics (Fermat's principle); antenna, cavity, and waveguide theories (Raleigh-Ritz, Rumsey, and Schwinger principles); laser/plasma and FEL physics (Hamilton's principle, least action principle); general numerical methods for electromagnetics (minimum residual, moment, finite-element, or Raleigh-Ritz-Galerkin methods), and specialized principles for FELs (e.g., Xie's principle)

(Also similar but not equivalent to the familiar Raleigh-Ritz approximation in quantum mechanics)

MPVP involves finding extrema of quantities of the form:

$$\mathcal{P} = -\,\mathrm{Re}\int d^3\boldsymbol{x}\,\boldsymbol{E}_{\mathrm{rad}}(\boldsymbol{x};\omega)^* \cdot \boldsymbol{J}(\boldsymbol{x};\omega)$$

while Rumsey's "reaction"-based variational principles would involve finding stationary points of quantities of the form:

$$\mathcal{R} = \mathrm{Re}\int d^3\boldsymbol{x}\,\boldsymbol{E}_{\mathrm{rad}}(\boldsymbol{x};\omega) \cdot \boldsymbol{J}(\boldsymbol{x};\omega)$$

is there another radiative reaction variational principle involving the imaginary part of this integral?

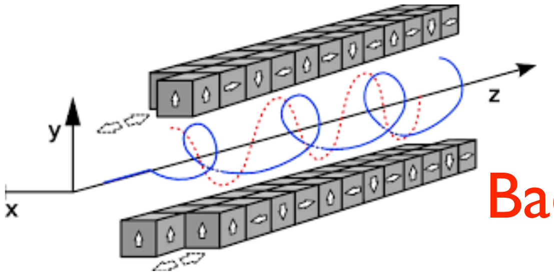
and Lagrangian action-based variational principles would involve finding stationary points of quantities of the form:

$$\mathcal{A} = \mathrm{Im}\int d^3\boldsymbol{x}\,\boldsymbol{E}_{\mathrm{rad}}(\boldsymbol{x};\omega)^* \cdot \boldsymbol{J}(\boldsymbol{x};\omega)$$

Because of the hyperbolic character of the wave equation, the stationary points of the action are generically saddle-points, rather than maxima/minima, so no bound on the radiated power can be directly obtained—in fact, if one attempts to use a "source-free" variational basis, the action-based principle becomes degenerate, and no absolute power level can be determined

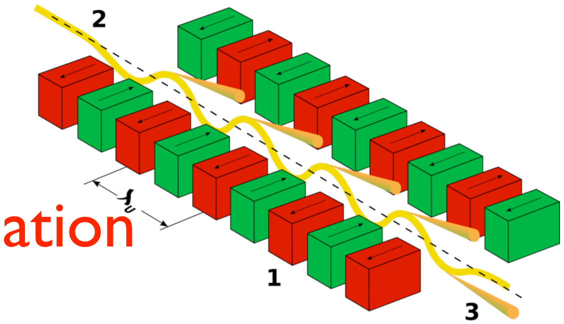
Some Further Comparisons

- *if* adjustable variational parameters appear as linear expansion coefficients in an orthonormal basis-set expansion, then MPVP reduces to two simple ideas:
  - **Bessel Inequality**: the EM power in any one source-free mode or finite superposition of orthogonal modes cannot exceed the power in all the modes
  - **Conservation of Energy**: power radiated must be attributable to power delivered by the sources, even when back-action is ignored and near fields remain unknown
- more generally, closest mathematical analog appears to be the *Lax-Milgram* theorem
  - which is the basis of Ritz-Galerkin and other finite element and spectral element numerical methods
  - but technical assumption assumptions of Lax-Mailgram theorem are not met
    - radiation kernel is *not* strictly *elliptic* and *coercive*
    - which is why solution space must be constrained to source-free solutions



Consistency Check:

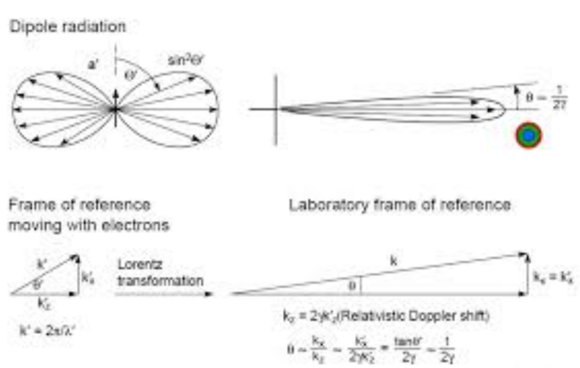
Back-Of-The-Envelope Undulator Radiation

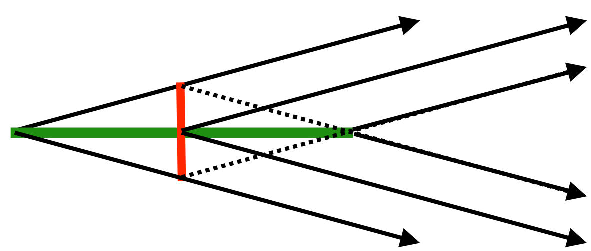


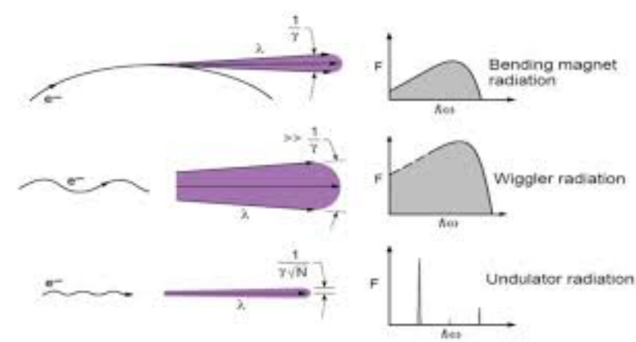
- consider "coherent mode" of radiation emitted by on-axis, low-emittance, highly mono-energetic, highly relativistic bunch in an ideal helical undulator with *a* < 1:
- peak wavelength estimated from resonance condition: $\lambda_1 \approx \frac{1+a_u^2}{2\gamma^2}\lambda_u$
- bandwidth estimated from time-frequency uncertainty principle $\frac{\Delta\omega}{\omega_1} \approx \frac{\sqrt{3}}{2\pi}\frac{1}{N_u}$
- transverse spot size, diffraction angle, Rayleigh range estimated via uncertainty principle and ray-tracing

$$\Delta\theta \approx \frac{1}{2\sqrt{\pi}}\frac{\sqrt{1+a_u^2}}{\sqrt{N_u}\gamma} \qquad \Delta r\,\Delta\theta \approx \frac{\lambda_1}{4\pi} \qquad z_R \approx \tfrac{1}{8}N_u\lambda_u$$

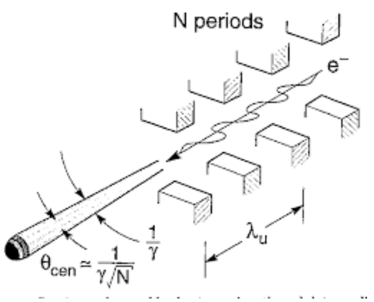
- photon emission estimated from Larmor formula in average rest frame $\mathcal{N}_c \approx \alpha\, a_u^2(1+a_u^2)$.





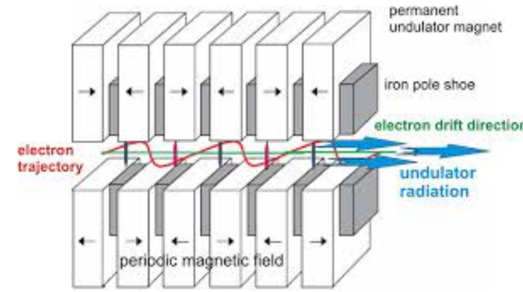


22



Consistency Check:

(semi-)analytical variational approximation



- as trial solution, use Gaussian paraxial mode with adjustable amplitude, phase, polarization, Rayleigh range, and waist location
  - still not tractable, so we make additional approximations, based on stationary-phase type argument and smallness of $a_u/\gamma \ll 1$
- peak wavelength and bandwidth estimated from stationary phase condition

$$\lambda_1 \approx \frac{1+a_u^2}{2\gamma^2}\lambda_u \qquad \frac{\Delta\omega}{\omega_1} \approx \frac{1}{N_U}$$

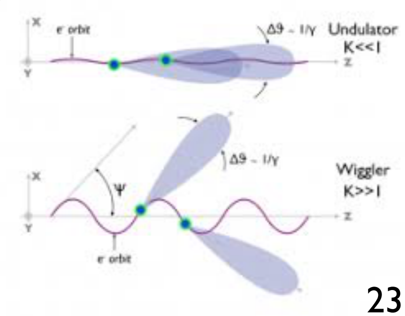
- Rayleigh range and waist location minimize $g(z_0, z_R; k_1) \approx k_1 z_R \left| \ln\left[\frac{z_0 - L_u + i z_R}{z_0 + i z_R}\right] \right|^2,$
  - implying

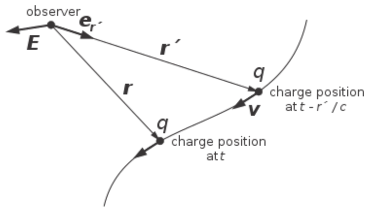
$$\frac{z_0}{L_u} = \frac{1}{2} \qquad \frac{2z_R}{L_u}\tan\left(\frac{4z_R L_u}{4z_R^2 + L_u^2}\right) = 1 \qquad \frac{z_R}{L_u} \approx 0.359261$$

- variational approximation energy emitted is $\mathcal{E}_c \approx \alpha\,\hbar\omega \frac{2a_u^2}{1+a_u^2}\frac{1}{\beta_z^2}\left(\frac{z_R}{L_u}\right)^3\left[\frac{8}{4\frac{z_R^2}{L_u^2}+1}\right]^2,$
  - with $\left(\frac{z_R}{L_u}\right)^3\left[\frac{8}{4\frac{z_R^2}{L_u^2}+1}\right]^2 \approx 1.29079$

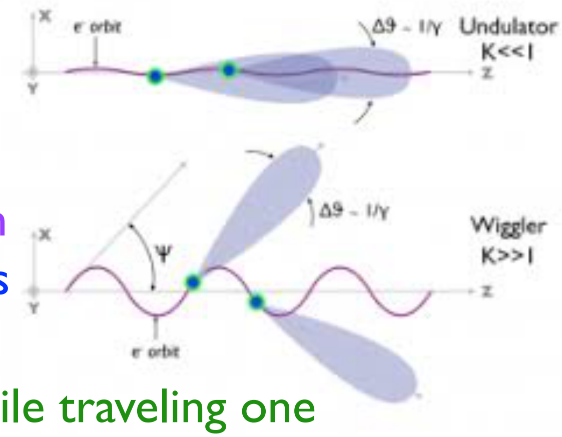
more-or-less consistent with earlier back-of-envelope calculations, but with some different pre-factors

and reconciles some “loopholes” in those arguments, regarding interference effects

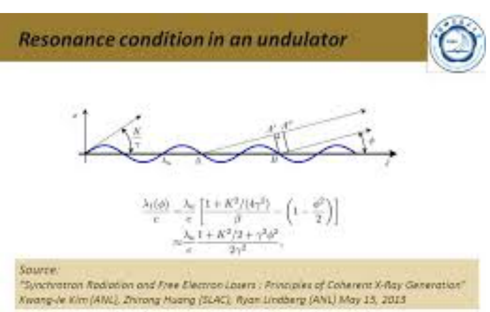


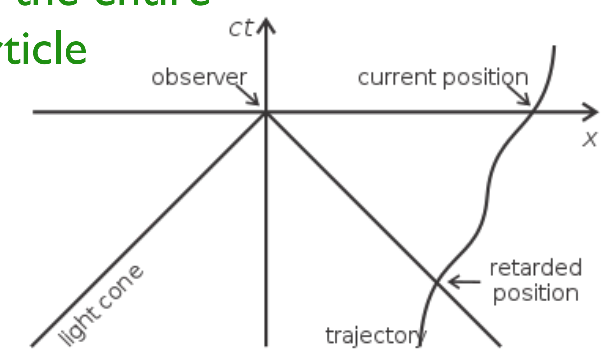


Closing a "Loophole"



- conventional arguments for both the peak (on-axis) emission wavelength and angular size of the central cone implicitly rely on interference effects
  - effectively treat electron beam approximately as a line source
  - resonate when electron slips behind radiation by one wavelength while traveling one undulatory period
  - emission angle smaller for undulator than wiggler because of overlapping cones
- but arguments do not really make sense for singe electrons
  - the past light cone of a given observation point can intersect any one electron's worldline at most once
  - so radiation emitted by one electron at different spacetime points cannot interfere
- of course, solving for Lienard-Wiechert fields, Heaviside-Feynman fields, or the like will verify that a single electron must radiate with the same intrinsic spectral and spatial pattern as does a beam of many electrons
- but MPVP also provides a simple verification
  - even one electron radiates as if to maximize energy exchange with the entire radiation mode, that extends upstream and downstream of the particle

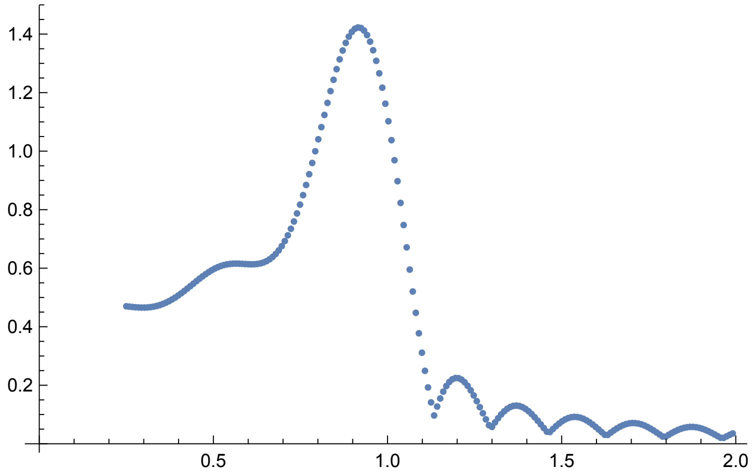


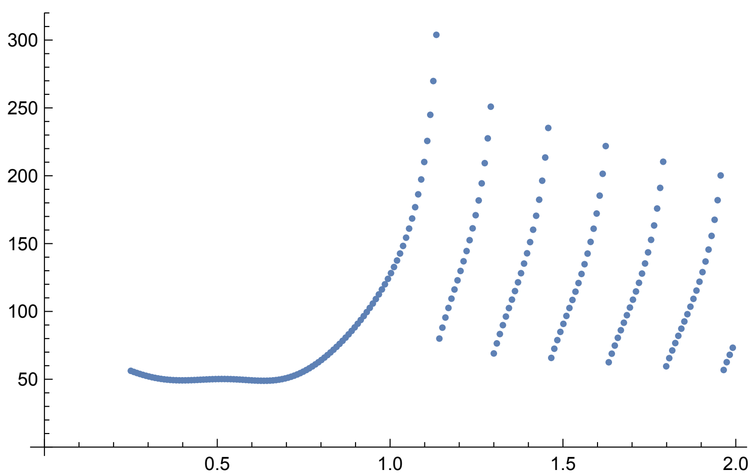


Consistency Check:

numerical variational approximation using Gaussian mode

output energy (arbitrary units)
vs. optical frequency (relative to resonance)





spot size (relative to optical wavelength)
vs. optical frequency (relative to resonance)

variational results are for one 100 MeV electron
in a helical undulatory with a_u = 0.8, N_u = 6, λ_u = 12.9 cm

trial solution was a single Gaussian paraxial mode,
with adjustable spot size but waist location fixed

but similar behavior when waist when
waist location is also varied

accuracy could be further improved by
including superpositions of additional modes

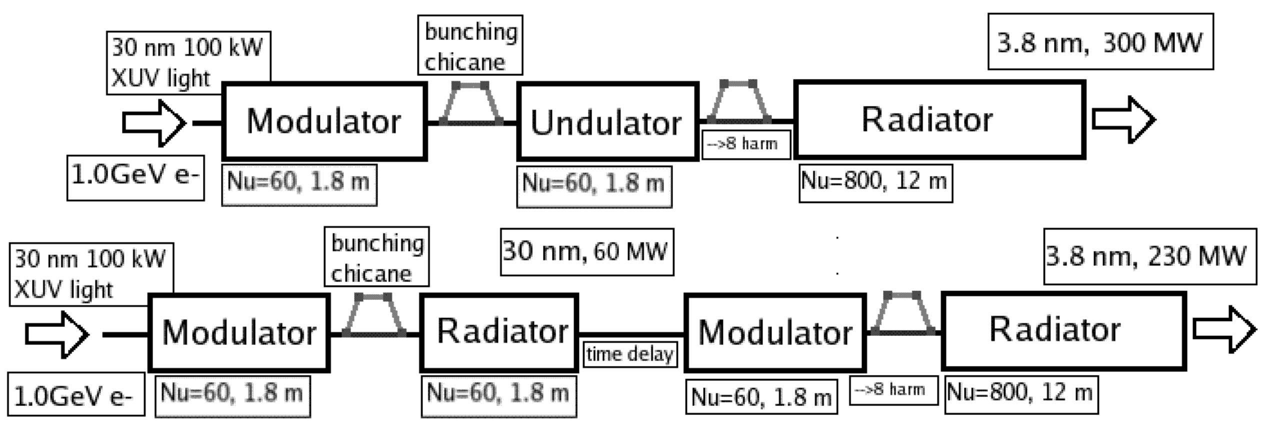
25

Applications to Harmonic Cascade FEL Radiation

Work at LBNL by G. Penn, J. Wurtele, M. Reinsch, A. Zholentz, B. Fawley, M. Gullans

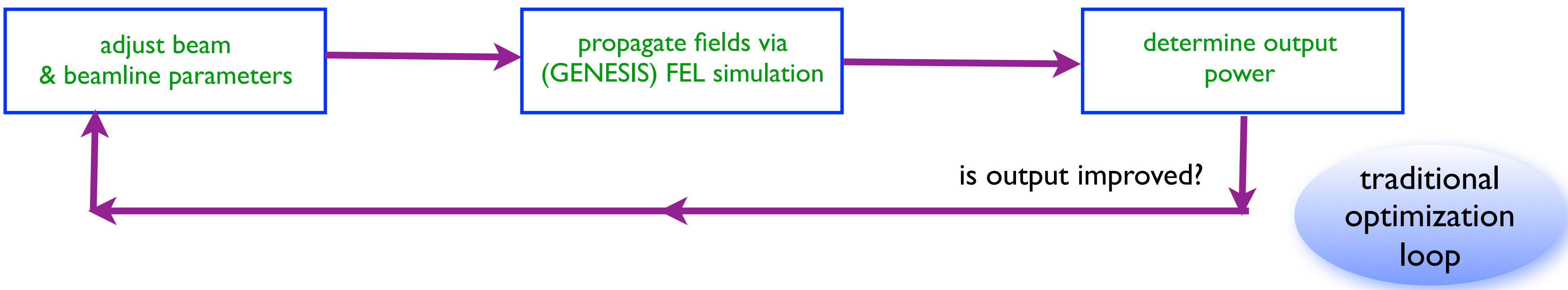
- In HHG proposal, multiple harmonic cascades in undulators results in high-brightness X-ray generation
    - **energy modulations** are introduced in an electron beam passing through a modulator-undulator while overlapping a seed laser, and are **converted into spatial modulations** (micro-bunching) via a specialized dispersive beam-line (chicane)
    - **bunching** occurs **at fundamental** and **higher harmonics** (due to nonlinearities), and beam is induced to radiate at chosen harmonic in a suitably-tuned second radiator-undulator
    - can be "**cascaded**:" **output radiation at** chosen harmonic can be **used as the seed in the next stage,** overlapping with a fresh part of the beam in a suitably-tuned downstream undulator to induce energy modulation at the higher frequency, and the process can be repeated....
    - if the gain is sufficiently low in each radiator-undulator, so that **prior bunching** from the modulator/chicane **dominates over self-bunching**, then the MPVP may be used to estimate the profile and power of the output radiation....

two typical proposed HHG-seeded configurations:

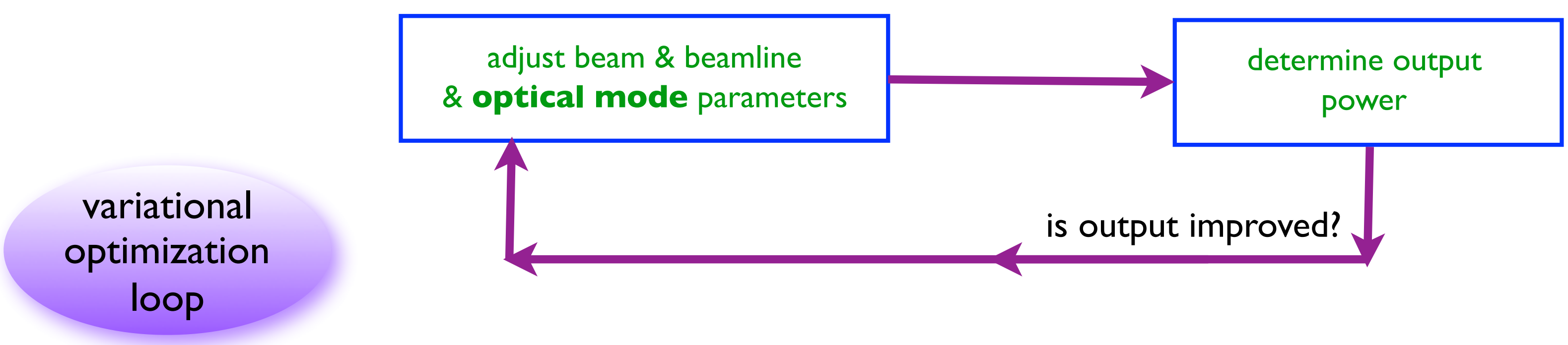


MPVP for HHG

- trial-function approach provides basis for efficient, analytic approximation tool for estimating radiation power and optimizing beam-line design
    - **far faster, simpler than lengthy FEL computer simulations** (GENESIS) or summation over single-particle fields, allowing for more economical parameter search for optimal design
    - **power-maximization over adjustable parameters in trial radiation mode may naturally be performed simultaneously with optimization over design parameters**, such as energy modulation, undulator strength, and chicane slippage factor....



versus

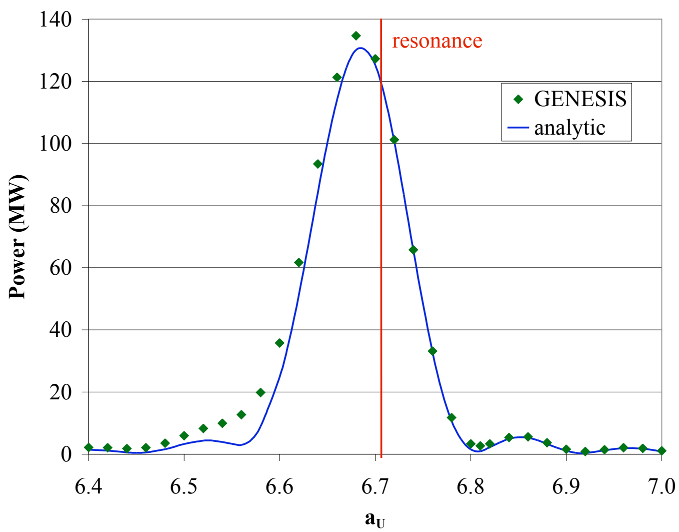


27

Harmonic Cascade: Results and Comparison

comparison of the analytic MPVP trial function approximation to to detailed numerical simulation (GENESIS code)

output power vs. undulator strength (50 nm)

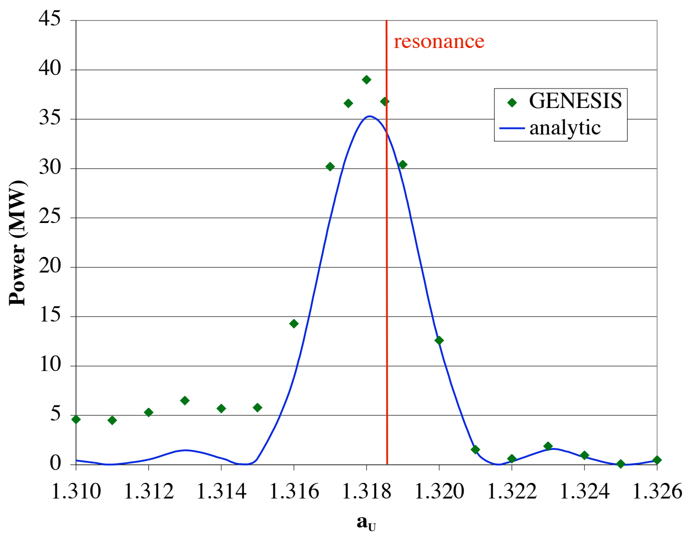


trial solution was a single Gaussian paraxial mode, with adjustable spot size and waist location

results are for 3.1 GeV, 2μ−emittance beams in single-stage radiators, producing (case a) 50 nm radiation (n = 4 harmonic) or (case b) 1 nm radiation (n = 3 harmonic)

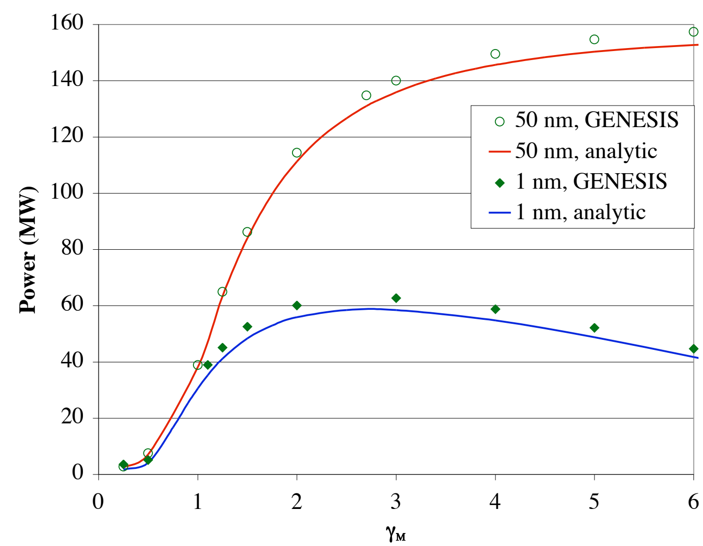
as expected, variational approximation systematically underestimates output power, by an average of 3% for 50 nm case and about 10% for 1 nm case

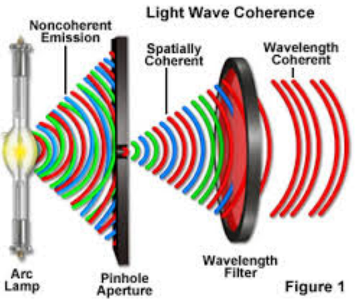
output power vs. undulator strength (1 nm)



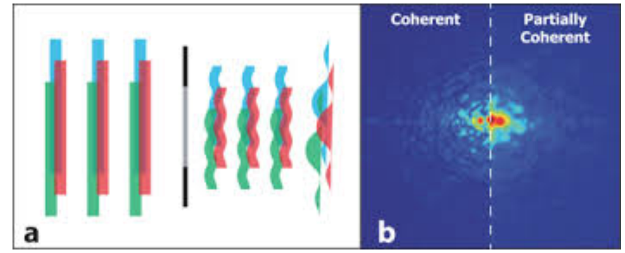
accuracy could be further improved by including additional modes, or by adding adjustable parameters to allow for ellipticity, annularity, skew or misalignment, kurtosis, etc., in radiation profile

output power vs.energy modulation

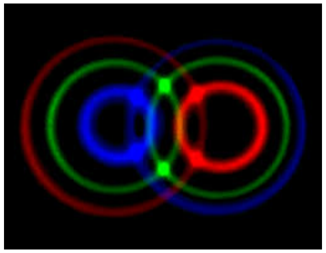




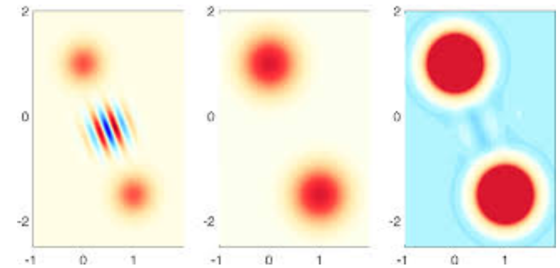
Partial Coherence



- uncertainty, randomness, jitter, fluctuations, finite emittance in sources will lead to partial coherence of radiation emitted
  - decreased degree(s) of coherence, interference fringe visibility, etc.
  - possibly decreased coherence times or longitudinal or transverse coherence lengths
  - and increased optical emittance
- any differences between classical and quantum radiation would mostly emerge in first-order or second-order coherence tensors
- but as formulated, simple application of MPVP will generate best coherent superposition over modes, not a statistical mixture
  - MPVP relates quantities both linear and quadratic in EM fields
  - so averaging over statistical uncertainty in electron bunch and optimizing with respect to variational parameters in trial fields do not commute
  - must be careful to distinguish averaged Poynting vector $\frac{1}{\mu_0}\langle \boldsymbol{E}(\boldsymbol{x},t) \times \boldsymbol{B}(\boldsymbol{x},t)\rangle$ from Poynting vector of averaged fields, $\frac{1}{\mu_0}\langle \boldsymbol{E}(\boldsymbol{x},t)\rangle \times \langle \boldsymbol{B}(\boldsymbol{x},t)\rangle$
- to capture effects of partial coherence, must optimize first, then average, rather than optimize on averaged source
  - but might there be some way to apply directly to coherence tensors instead of fields?
  - also possible to Weyl transform paraxial modes to assess correlations in "wave-kinetic" phase-space, as emphasized by K-J. Kim



Quantum Optical Effects?



- As formulated, MPVP applies to situations where sources are assumed to be *prescribed* *C*-number currents
  - or equivalently, as point charges following prescribed spatiotemporal trajectories
- coincides exactly with class of sources that lead to classical radiation fields according to conventional criterion in quantum optics
  - corresponding to non-negative Glauber-Sudarshan quasi-distribution functions
- but resulting approximate modes may be convenient starting point for exploring possible quantum optical effects
  - e.g., using paraxial "wave-packet quantization" formalism of Garrison. Deutsch, and Chiao
  - just replace c-number paraxial fields with corresponding wave-packet operators
- to look for (hard to see!) quantum effects such as
  - sub-Poissonian statistics, photon anti-bunching, or other inter-arrival statistics
  - Hong-Ou-Mandel (HOM) interference, non-classical Hanbury-Brown-Twiss effects, etc.
  - other angular or spatial correlations or entanglement
  - violation of Leggett-Garg or Bell-Clauser-Horne-Shimony-Holt type inequalities

30

Summary of MPVP

- mathematical details aside, the maximum-power variation principle is a straightforward consequence of simple ideas:
  - **radiation fields “look as much as possible” like the sources that emit them** (consistent with the fields being superpositions of source-free solutions to Maxwell’s equations)
  - **charges “radiate as much as possible” consistent with with energy conservation** (power radiated must be attributable to power delivered by the sources, even when back-action is ignored and near-fields remain unknown)
  - **Maxwell equations imply useful connections between “Joule” inner products involving radiation fields and “Poynting” functional inner products for outgoing far-fields** (sources transfer energy irreversibly only to radiation fields, and energy exchange be calculated as if all and only radiation fields are present in vicinity of sources)
- however intuitive or even trivial, these connections are not without practical consequences:
  - successfully applied to the problem of spontaneous undulator radiation and low-gain FELs
  - potential for wider applicability
- resulting approximations inherit the usual advantages and disadvantages of extremal variational approaches:
  - energy estimate is comparatively insensitive to errors in trial mode (2nd-order in “shape” errors)
  - but provides only a lower-bound
  - field profile/shape is approximated with comparatively less accuracy than is energy or power
  - but approximation can be systematically improved by including more parameters
  - amenable to more efficient analytic or numerical calculation, particularly in paraxial regime

Future Directions and Extensions

- generalization to stochastic or statistical emission?
  - move beyond mere averages for sources of finite emittance and deviations
  - **incoherent or partially coherent light?**
  - can we optimize directly via coherence tensor and van Cittert-Zernicke theorem
  - or Wigner function/phase-space representation
- another reaction-like variational principle to complete the family?
  - and is it useful for anything?
- structured, inhomogeneous, or nonlinear media?
  - dielectric structures?
  - waveguides and beam-pipes? CSR or OTR?
  - exotic photonic bandgap (PBG) materials?
- high-gain FELs or other systems?
  - perturbative or iterative approach for moderate gain?
  - connection to other generalizations or variations of Madey's Theorem?
- applicable in quantum optical regimes?
  - accommodate density operators with negative Glauber-Sudarshan *P* representations?
  - possibly relevant to IOTA experiments on radiation from very small e^- bunches